

Cyclohexanol
108-93-0 | DTXSID4021894

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 9.28e-01 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.15e-01

Confidence level: 8.49e-01

Nearest Neighbors from the Training Set

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1,3,5-Trichlorobenzene

Measured: 8.00e-01

Predicted: 4.17e-01

Image not found

Methyl chloroacetate

Measured: 2.49

Predicted: 11.6

Image not found

4-Methylheptane

Measured: 9.89e-01

Predicted: 22.4

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3,5-Dimethylpyridine

Measured: 4.79e-01

Predicted: 9.36e-01